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University of Idaho

Precompound Emission of Energetic Light Fragments in Spallation Reactions

Dissertation Proposal by Leslie M. Kerby

Major Professor: Akira T. Tokuhiro, Ph.D.

Los Alamos National Laboratory Mentor: Stepan G. Mashnik, Ph.D.

Feb 27, 2014

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Outline

- Introduction
- Why This Research Is Important
- Spallation Reaction Models
- Statement of Project
- Limitations
- Skills and Tools Required
- Timeline
- Summary

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Introduction

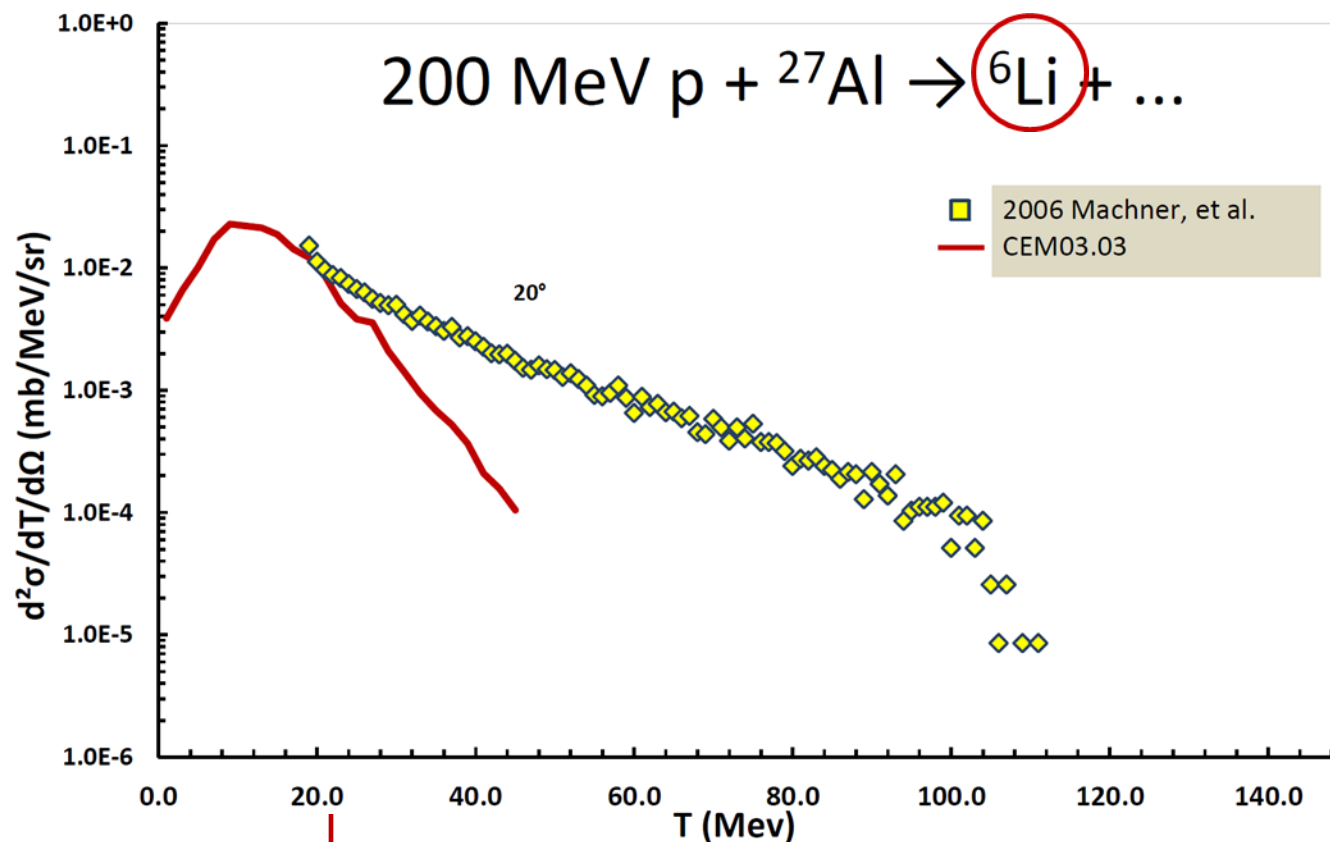
- Emission of energetic light fragments (LF) from nuclear reactions is an open question:
 - Different reaction mechanisms contribute
 - Relative roles of each not fully understood
 - Dependence on incident energy, target mass number, type and energy of fragment, not fully understood
- None of the available models are able to predict emission of energetic LF from arbitrary reactions;
- Cascade Exciton Model (CEM) and Los Alamos Quark-Gluon String Model (LAQGSM) predict the spectra of fragments up to ^4He well, and low-energy LFs;

Aim of our work is to extend CEM and LAQGSM for a more accurate prediction of high-energy LF by Monte Carlo N-Particle Transport Code version 6 (MCNP6).

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Introduction, cont.



Machner et al., PHYS. REV. C 73 (2006) 044606.

Evaporation

Precompound

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- # Setup
-
- Beam
- 100°
- 65°
- 35°
- 15°
- 20°
- 50°
- 80°
- 120°
- L1, L2, L3, L4, L5, L6, L7, L8 – phoswich detectors
- F1, F2 – cooled Si-telescopes
- E1, E2 – bragg curve detectors with Si-detectors
- B1, B2, B3, B4 – multichannel plates
- H1, H2 – beam monitors telescopes
- V1, V2 – cosy valves
- C1, C2 – high vacuum protecting foils
- (a)

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Why This Research Is Important



Single Event Upsets (SEUs)

- **October 2008, Airbus en route from Perth to Singapore¹**

¹Necia Grant Cooper, "The Invisible Neutron Threat", National Security Science Feb. 2012: 13.

- **Satellite computer chip malfunctions cause false alarms²**

²A. Borning, *Computer System Reliability and Nuclear War*, (Foundation for Global Community, 1987).

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Why This Research Is Important, cont.

Also Important in

- Radiation Shielding¹
- Medical applications (proton and ion therapy for cancer)²
- Understanding better the mechanisms of nuclear reactions

¹R. Singleterry, Space Travel and the Long Tent Pole, presentation at LANL, San Ildefonso Auditory, August 2012, and private communication from Dr. Singleterry, 2012.

²N. MacReady, The Promise of Protons in Cancer Therapy, Journal of the National Cancer Institute 104(9) (2012).

The 2008-2010 IAEA Benchmark of Spallation Models

- Recommended considering preequilibrium emission (and maybe also coalescence production) of fragments heavier than ^4He ^{3,4}

³S. G. Mashnik et al., “Second Advanced Workshop on Model Codes for Spallation Reactions”, CEA-Saclay, France, 8-11 Feb 2010, LA-UR-10-00510.

⁴S. Leray et al., “Results from the IAEA Benchmark of Spallation Models”, Journal of the Korean Physical Society Vol. 59, No. 2 (2011), 791-796.

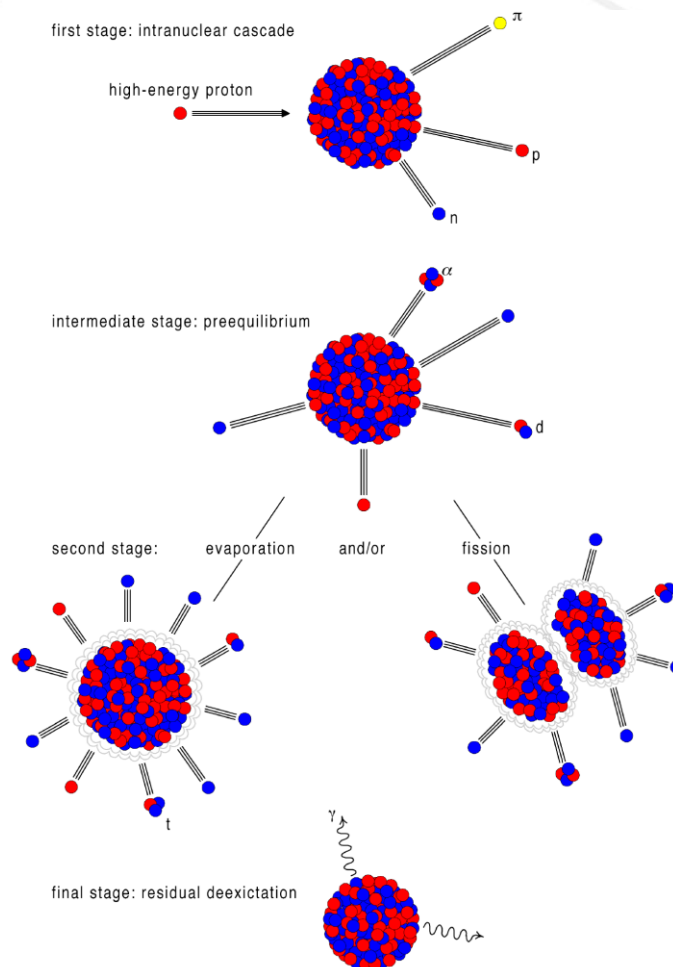
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Spallation Reactions

Precompound

Compound

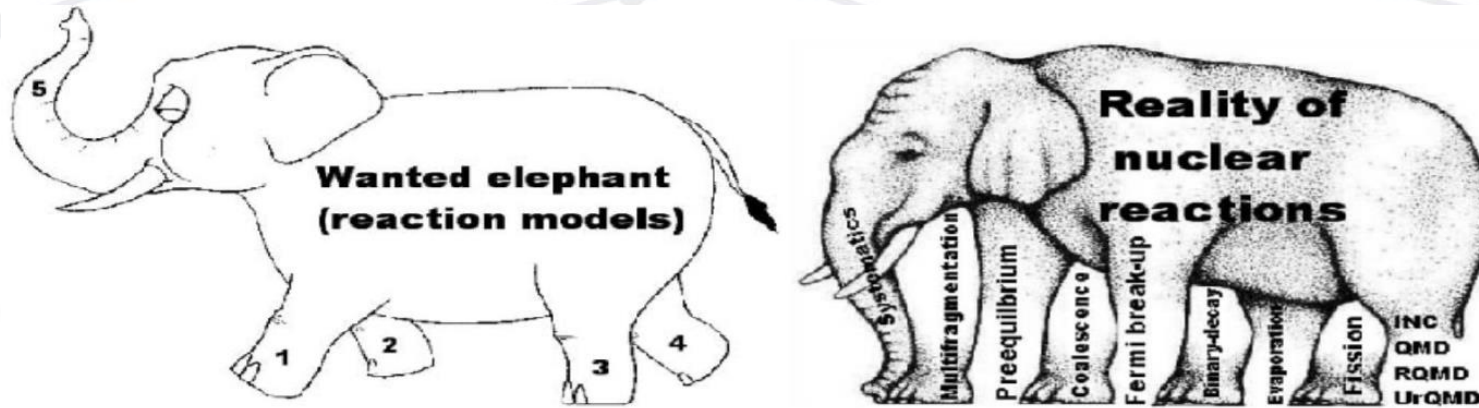


Adapted from: S. Mashnik, "High Energy Model Physics," MCNP Class Lectures.

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Spallation Reaction Models



(Adopted from: S. G. Mashnik et al., LA-UR-10-00510, 2d Advanced Workshop on Model Codes for Spallation Reactions, 8-11 February 2010, CEA Saclay, France)

Precompound Codes:

- CEM/LAQGSM
- INCL
- QMD
- Isabel INC
- Bertini INC
- ALICE/INPE, Obninsk
- Y. Uozumi et al., 2007

■ SMM

■ Coalescence

Compound Models:

- GEM2
- ABLA
- ...
- Fission
- Fermi break-up

Transport codes:

- MCNP6
- GEANT4
- PHITS
- FLUKA
- MARS
- SHIELD
- ...

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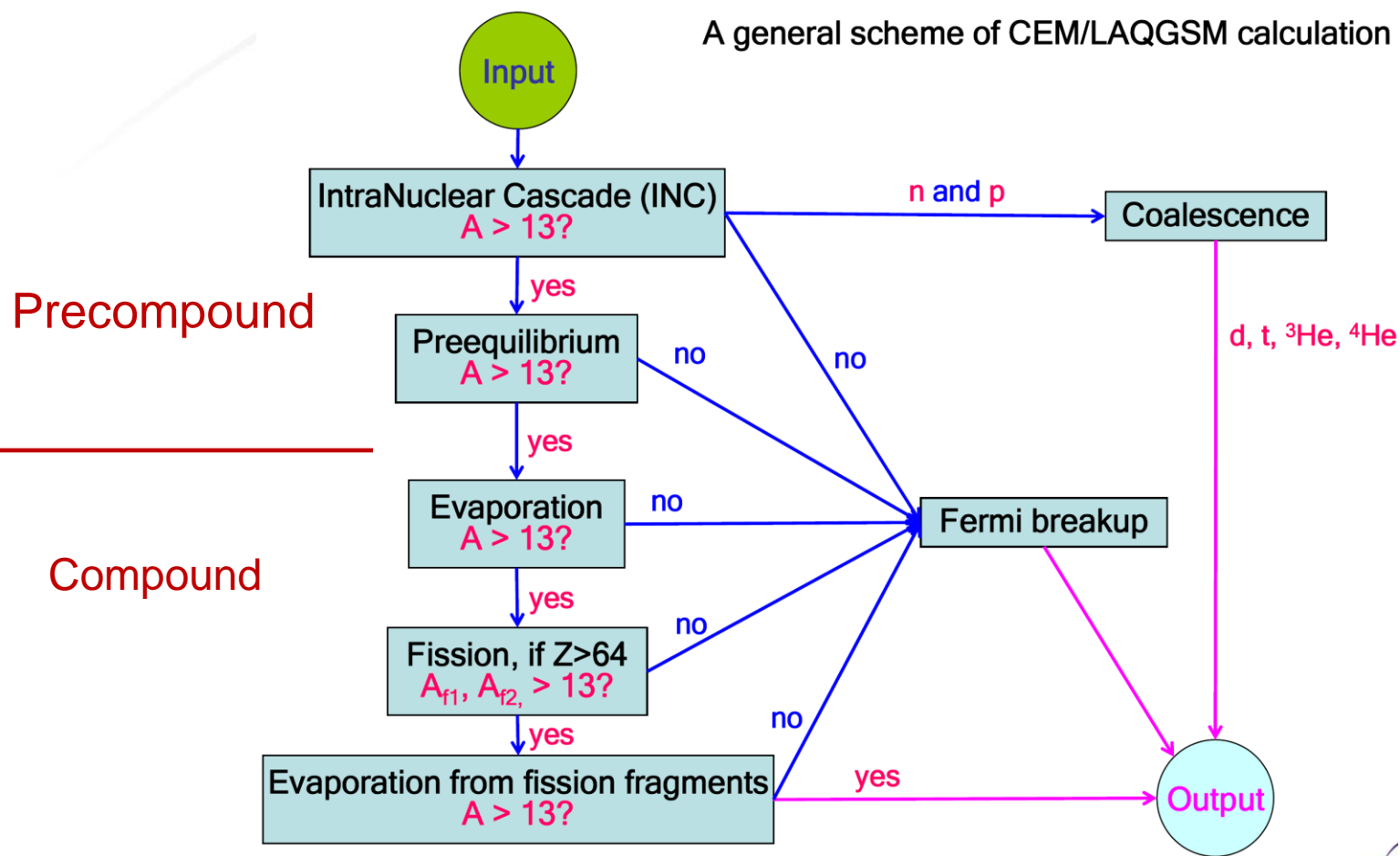
Comparison of Models providing LF

Model	Strengths	Weaknesses	Notes
CEM	Photonuclear, speed, accuracy	N-, π -, and γ - induced reactions only	LANL: S. G. Mashnik and A. J. Sierk, CEM03.03 User Manual, LANL Report, LA-UR-12-01364, ...
LAQGSM	A+A, any particle and any energies up to ~1 TeV/nucleon	Less accurate at low energies, <1 GeV	LANL: K. K. Gudima, S. G. Mashnik, and A. J. Sierk, User Manual for the code LAQGSM, LANL Report LA-UR-01-6804, ...
INCL	Nucleon and light ions induced reactions, accuracy	No photonuclear, no heavy-ions, and no high energies	Liege University, Belgium: A. Boudard, J. Cugnon, S. Leray, and C. Volant, Phys. Rev. C66 (2002) 044615, ...
QMD	Physics, heavy ion interactions	Slow, not as accurate (so far)	Europe, Japan, ... K. Niita, S. Chiba, et al., Phys. Rev. C52 (1995) 2620; S. A. Bass et al., Prog. Part. Nucl. Phys. 41 (1998) 255, ...
ALICE/INPE	Used to produce data libraries for applications	< 200 MeV	Obninsk, Russia: A. Yu. Konobeev and Yu. A. Korovin, Kerntechnik 60 (1995) 147; A. I. Dityuk, et al., Report INDC(CCP)-410, IAEA, Vienna (1998), ...

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Cascade Exciton Model

A general scheme of CEM/LAQGSM calculation



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Modified Exciton Model (within CEM)

The Modified Exciton Model (MEM) used by CEM⁵ calculates Γ_j , the emission width (or probability of emitting particle fragment j) as

$$\Gamma_j(p, h, E) = \int_{V_j^c}^{E-B_j} \lambda_c^j(p, h, E, T) dT \quad (1)$$

where the partial transmission probabilities, λ_c^j , are equal to

$$\lambda_c^j(p, h, E, T) = \frac{2s_j + 1}{\pi^2 \hbar^3} \mu_j \Re(p, h) \frac{\omega(p-1, h, E - B_j - T)}{\omega(p, h, E)} T \sigma_{inv}(T) \quad (2)$$

For complex particles, an extra factor γ_j is introduced:

$$\gamma_j \approx p_j^3 \left(\frac{p_j}{A} \right)^{p_j-1} \quad (3)$$

⁵K. K. Gudima, S. G. Mashnik, and V. D. Toneev, "Cascade-Exciton Model of Nuclear Reactions," Nuclear Phys. A401 (1983) 329-361.

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Statement of Project

1. Modify CEM code to emit 66 particles and light fragments (vs 6 originally) in the preequilibrium modules;
2. Parameterize γ_β for ~ 100 proton spallation reactions;
3. Parameterize γ_β for ~ 50 neutron spallation reactions;
4. Analyze γ_β parameterization for a possible physical/mathematical model;
5. Re-write γ_β CEM modules to either incorporate the new mathematical model or utilize modern interpolation and extrapolation methods using our parameterization;
6. Investigate Fermi break-up model expansion;
7. Investigate coalescence model expansion;
8. Replace the MEM in LAQGSM with our expanded MEM and test;
9. Extend GENXS option of MCNP6 to tally arbitrary products and test;
10. Replace upgraded CEM, LAQGSM, and GENXS modules in MCNP6 and test.

Original Research Contribution: Expand preequilibrium processes to include emission of light fragments and create systematics (or mathematical model) for generalization across arbitrary reactions.

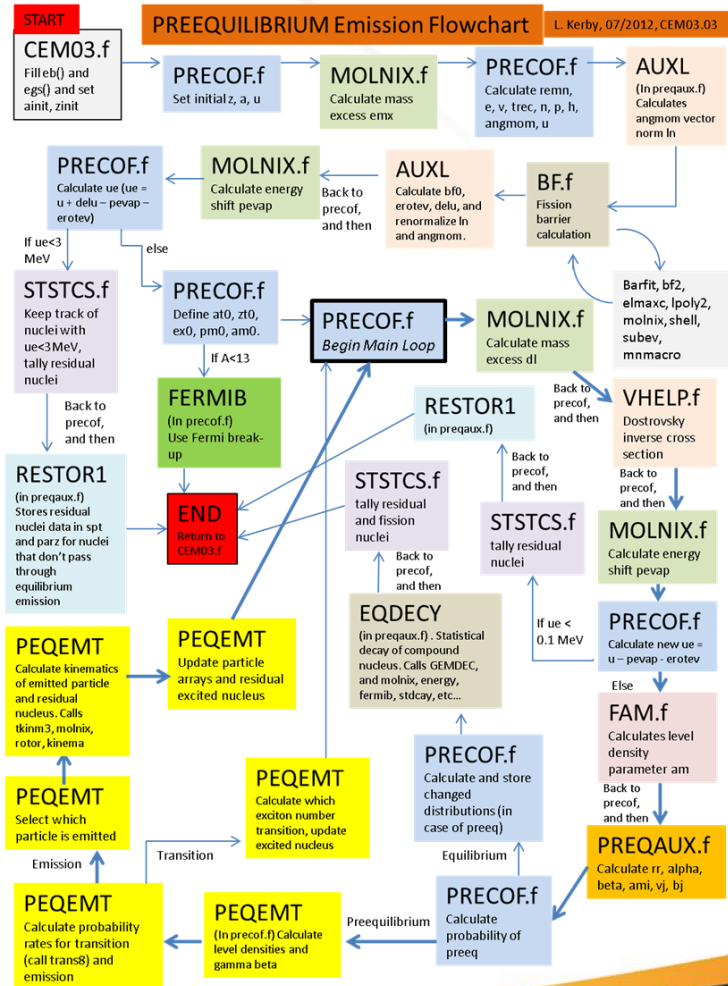
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1. Modify CEM code to emit 66 particles in the preequilibrium modules

- Modifications to many subroutines
- Testing
- Bug fixing

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2. Parameterize γ_β for proton reactions

$$\gamma_j \approx p_j^3 \left(\frac{p_j}{A} \right)^{p_j-1}.$$

Introduce a parameter F_j :

$$\gamma_j = F_j p_j^3 \left(\frac{p_j}{A} \right)^{p_j-1}.$$

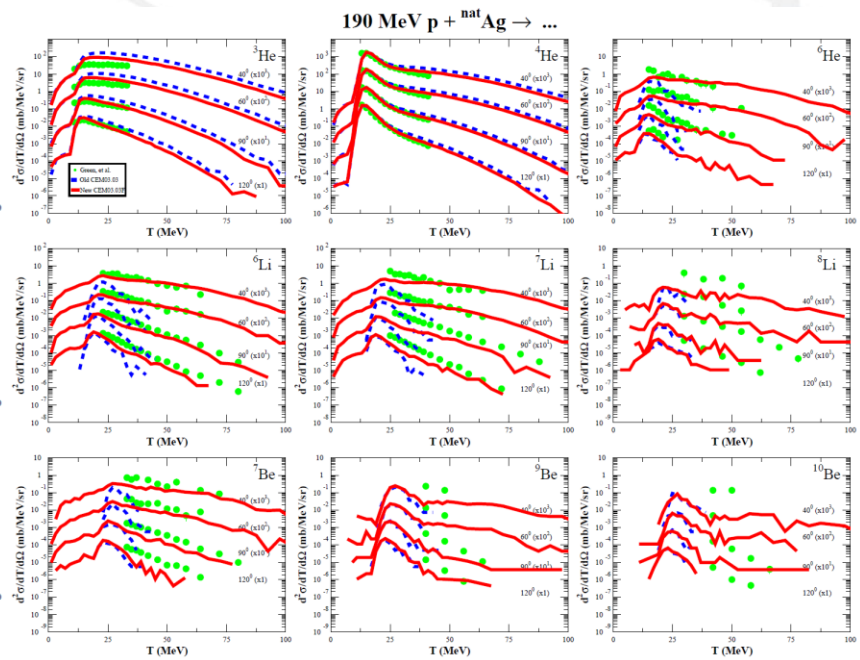
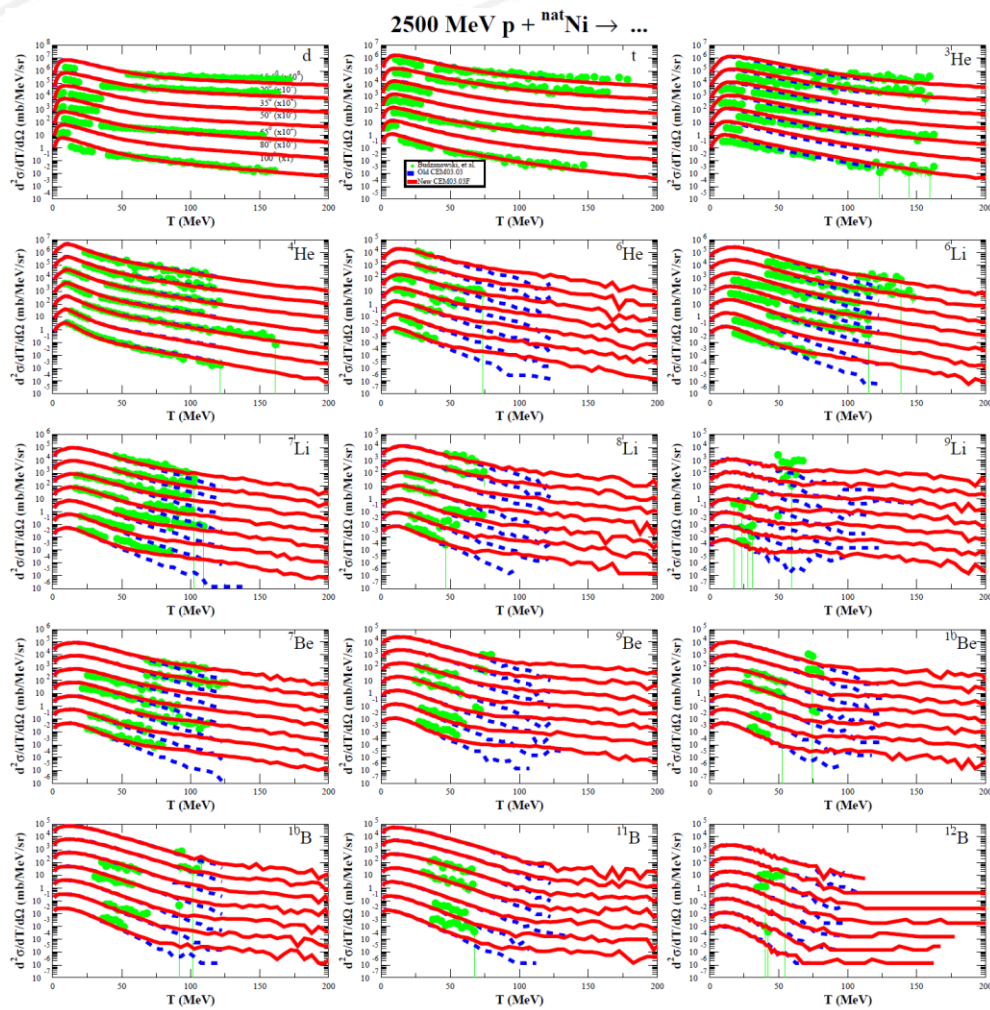
This parameter should be fit for as many different

- Target nuclei
- Incident energies
- Emitted light fragments

as possible (as we have reliable experimental data for).

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Results

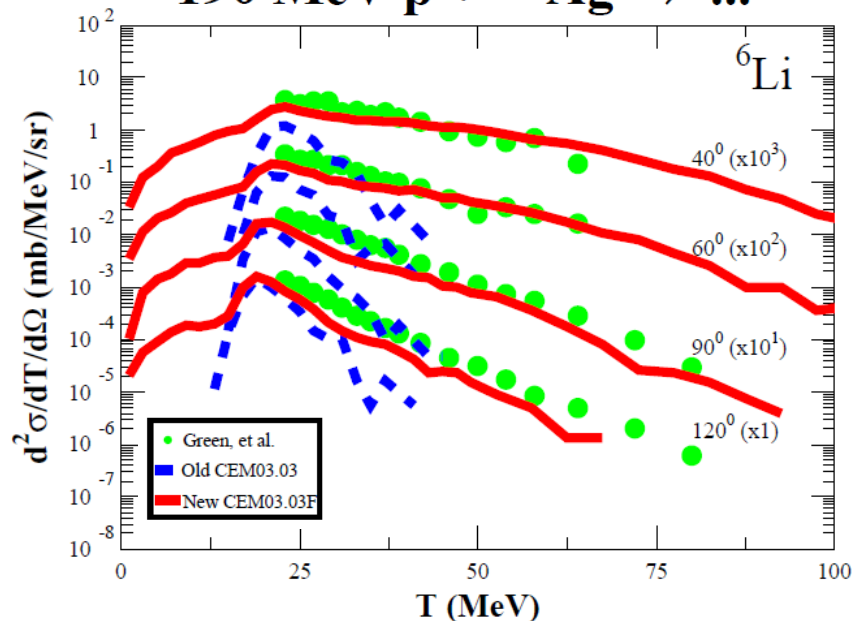


And many more...

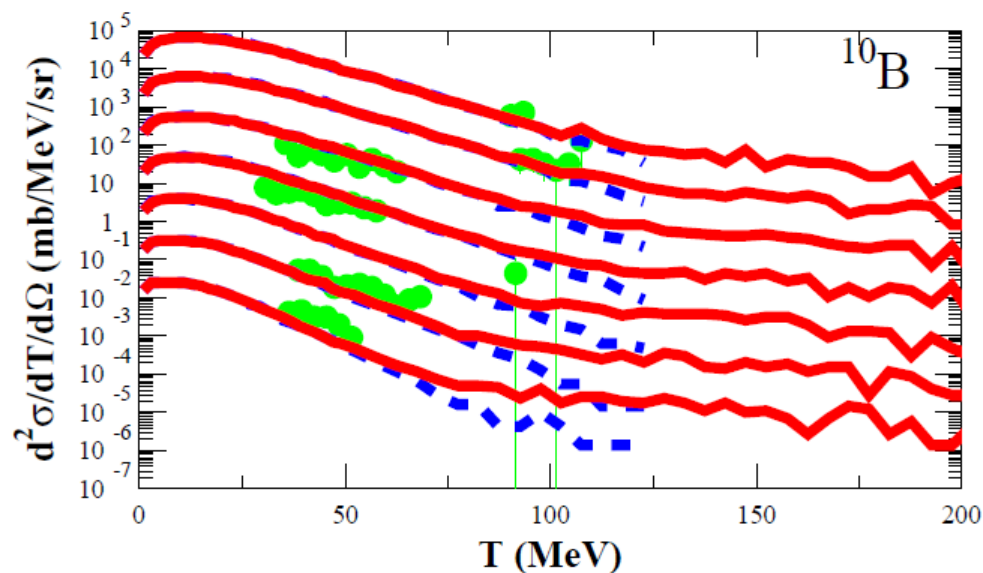
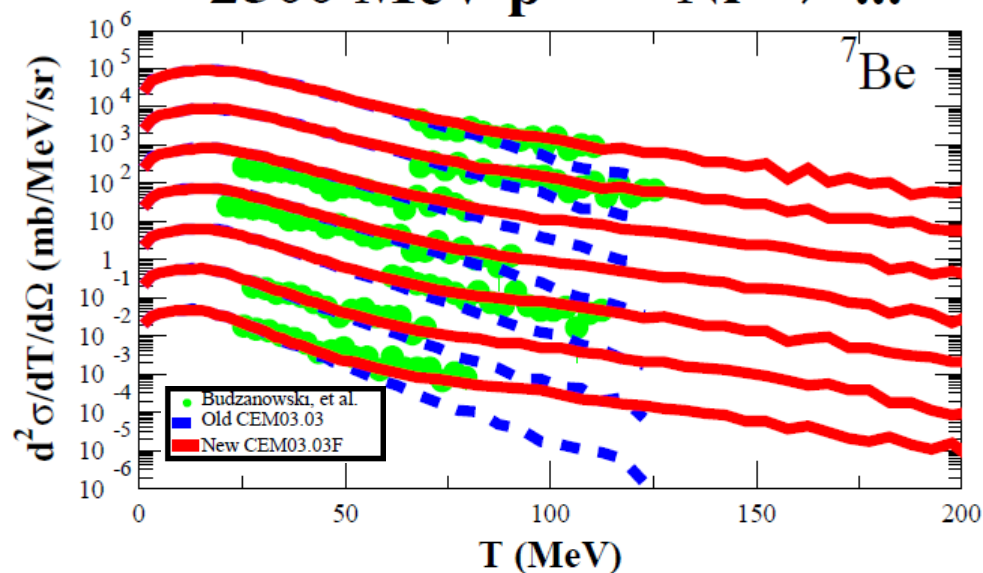
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Results, cont.

190 MeV p + ^{nat}Ag → ...



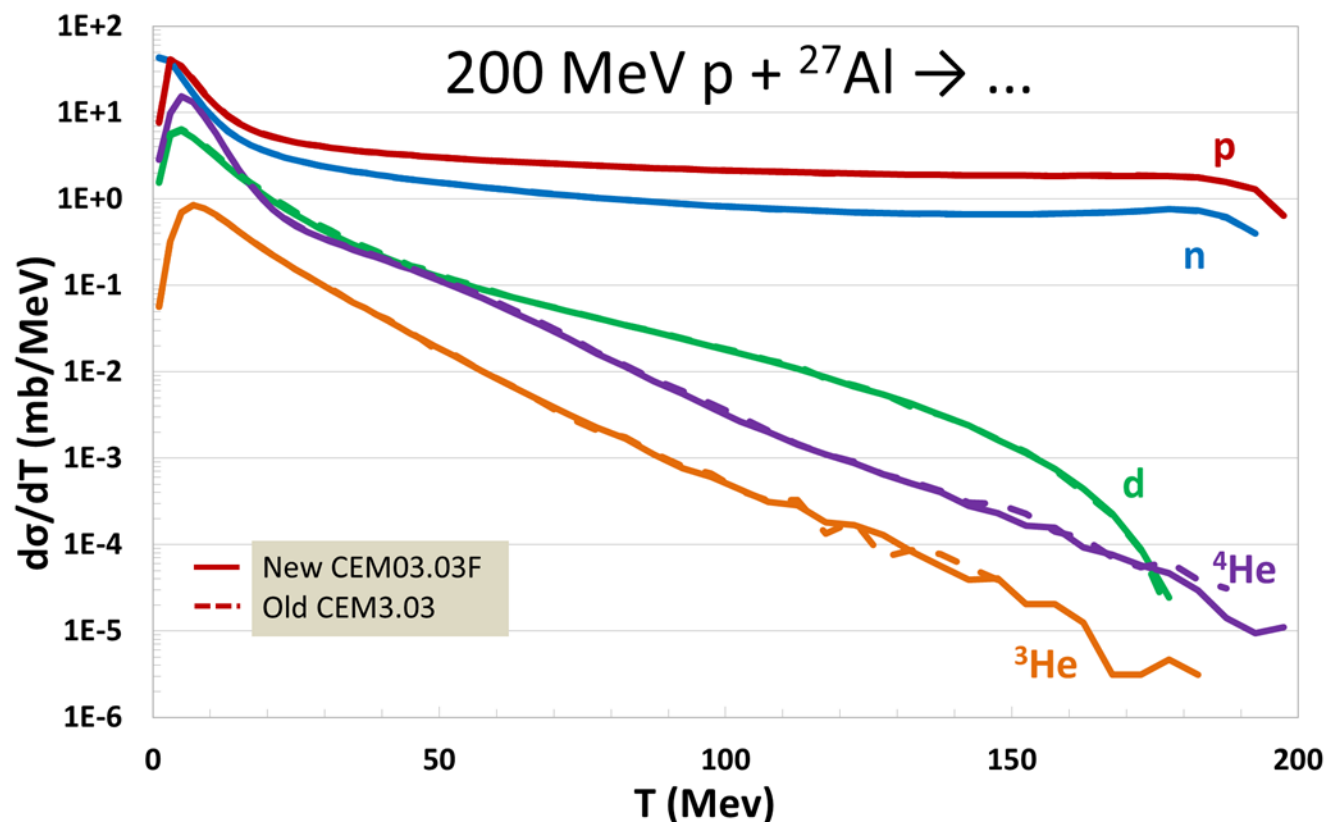
2500 MeV p + ^{nat}Ni → ...



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Results: Integral Spectra Preserved



High-energy tails of light fragments were obtained without changing significantly spectra of n, p, d, t, ^3He , and ^4He

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3. Parameterize γ_β for neutron reactions

- Once we are done parameterizing γ_β for the proton-induced reactions, we need to do the same thing for neutron-induced reactions. There are fewer experimental data of these.

4. Analyze γ_β parameterization for a possible physical/mathematical model

- Using our parameterization we will try to find a physical or mathematical model for γ_β ;
- Otherwise use systematics;
- Or combination.

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Develop Model (Step 4 cont.)

Table 2: F_j values for 200 MeV p + ^{27}Al

n	p	d	t	^3He	^4He	^6He	^8He	^6Li	^7Li
1.0	1.0	2.0	4.0	20.0	30.0	1.0	1.0	5.0	2.0
^8Li	^9Li	^7Be	^9Be	^{10}Be	^{11}Be	^{12}Be	^8B	^{10}B	^{11}B
1.7	10.0	0.3	0.2	0.2	0.2	0.2	0.2	0.2	0.1
^{12}B	^{13}B	^{10}C	^{11}C	^{12}C	^{13}C	^{14}C	^{15}C	^{16}C	^{12}N
0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
^{13}N	^{14}N	^{15}N	^{16}N	^{17}N	^{14}O	^{15}O	^{16}O	^{17}O	^{18}O
0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
^{19}O	^{20}O	^{17}F	^{18}F	^{19}F	^{20}F	^{21}F	^{18}Ne	^{19}Ne	^{20}Ne
0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
^{21}Ne	^{22}Ne	^{23}Ne	^{24}Ne	^{21}Na	^{22}Na	^{23}Na	^{24}Na	^{25}Na	^{26}Na
0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
^{23}Mg	^{24}Mg	^{25}Mg	^{26}Mg	^{27}Mg	^{28}Mg	^{29}Mg	^{30}Mg	^{31}Mg	^{32}Mg
0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1

$E^* = 35.0 \pm 33.5 \text{ MeV}$

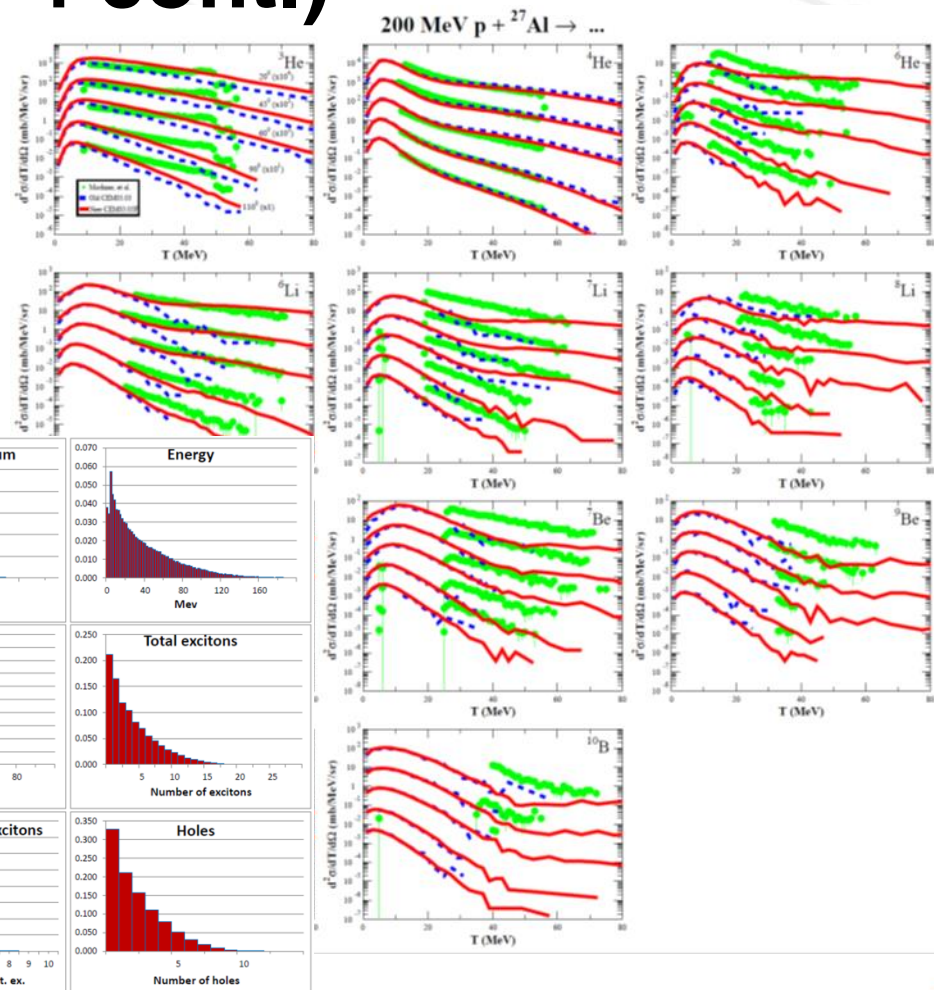
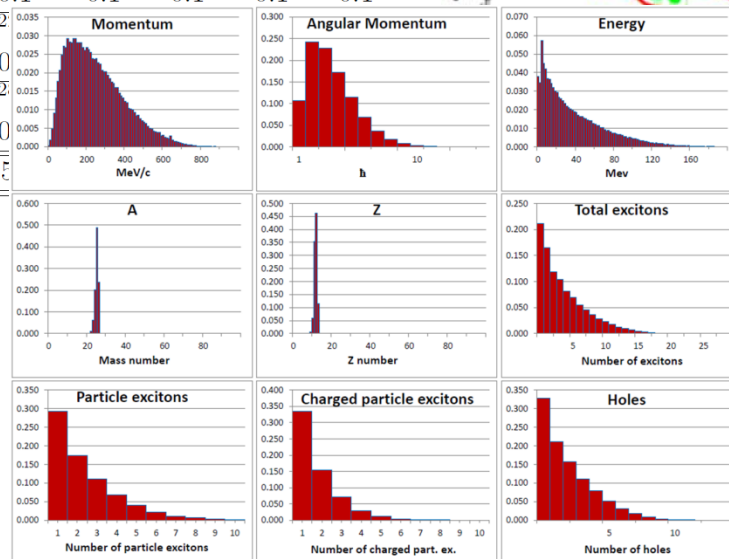
$Z = 12.5$

Target: ^{27}Al

Projectile: p

Incident energy:
200 MeV

Probability



Residual nuclei properties

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5. Re-write γ_β modules to incorporate step 4 model

From step 4 we will have

- A physical or mathematical model (hopefully)
- Systematics
- Or a combination.

We'll use this to re-write the γ_β modules in Fortran 90, incorporating modern interpolation and extrapolation methods.

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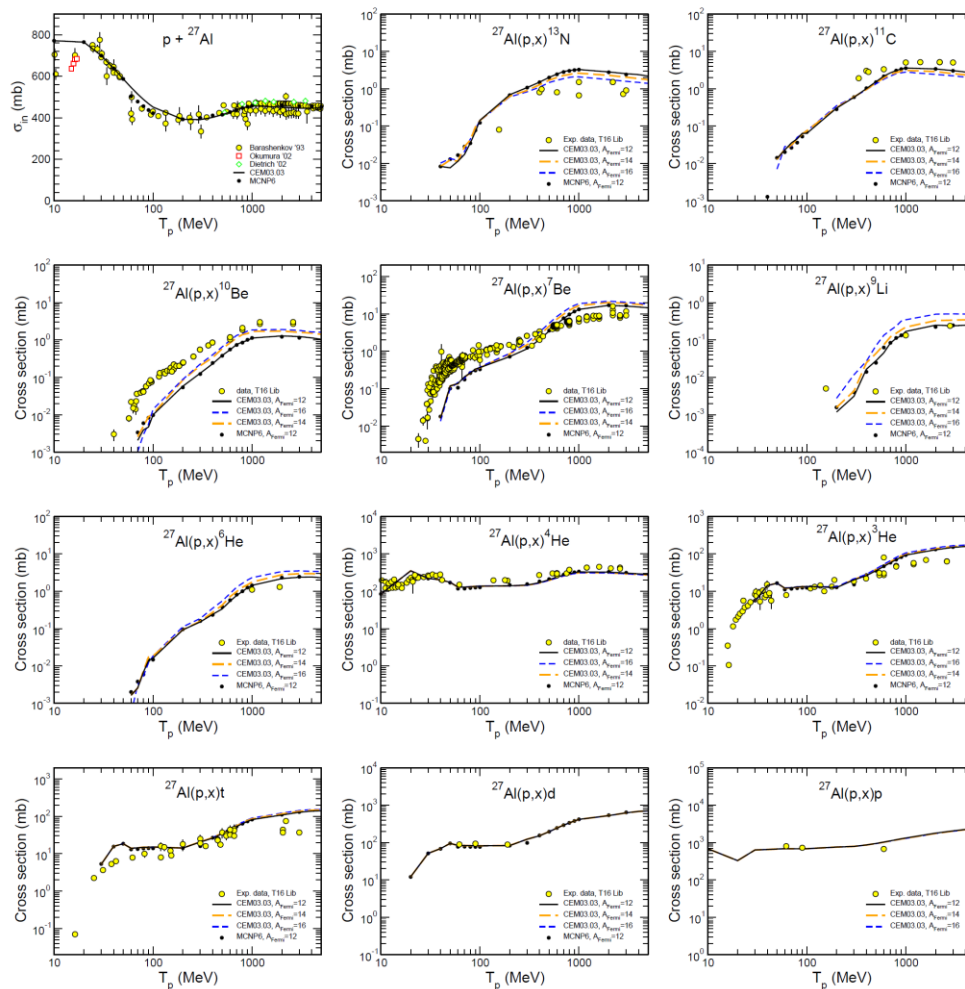
6. Investigate Fermi Break-up

- Currently CEM uses Fermi break-up when the residual nucleus has $A < 13$
- The best cut-off value has never been studied
- We are considering cut-off values of $A=12$, $A=14$, and $A=16$

Initial results:

$A=16$ better for heavier LF

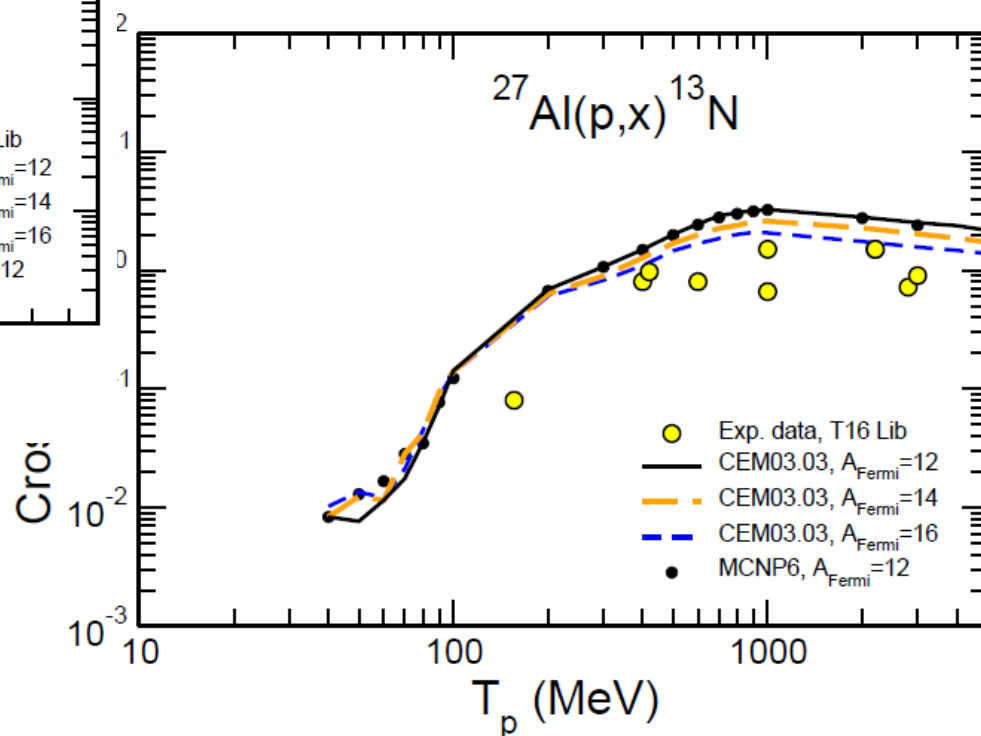
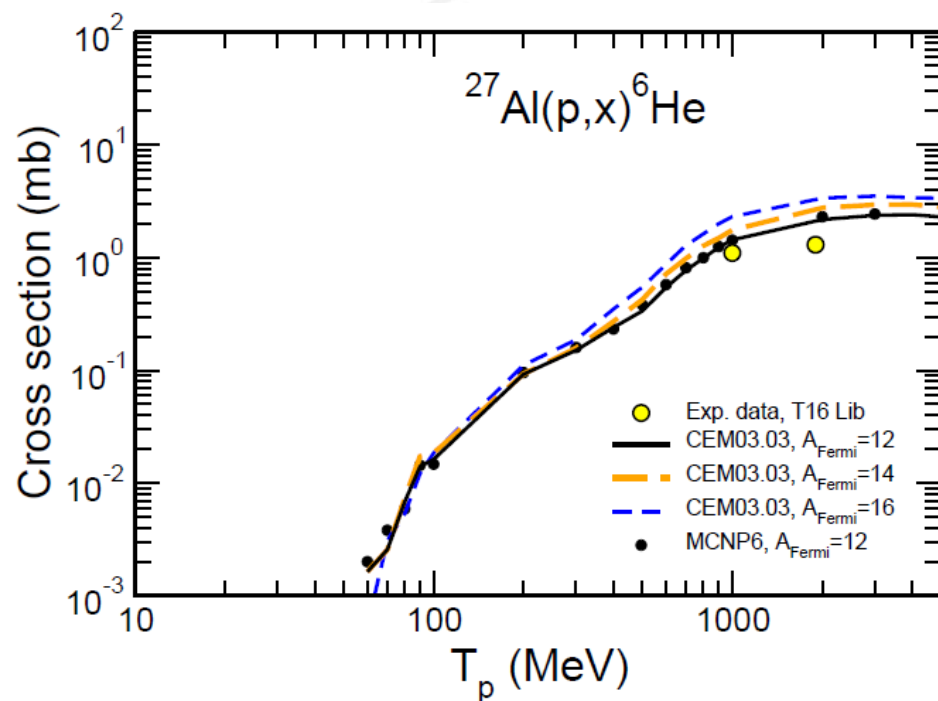
$A=12$ better for lighter LF



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Fermi Break-up, cont.



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7. Investigate Coalescence

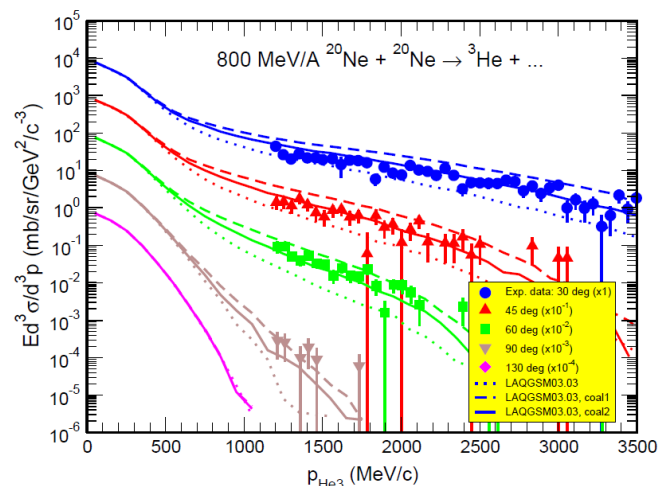
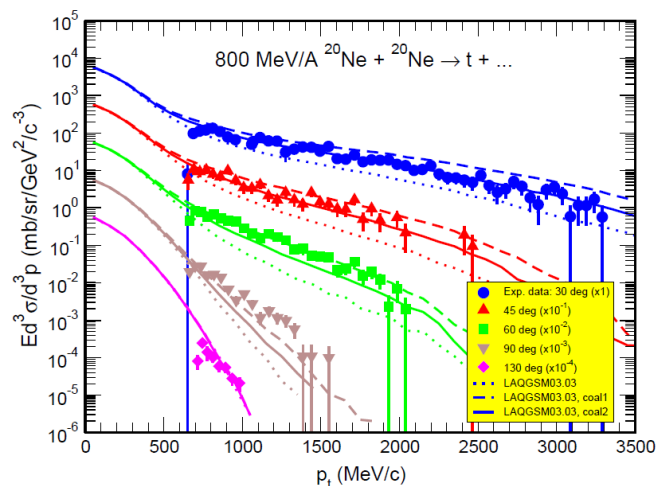
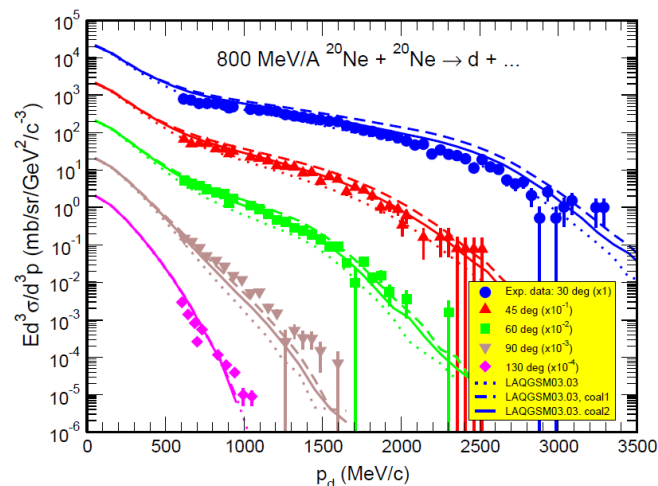
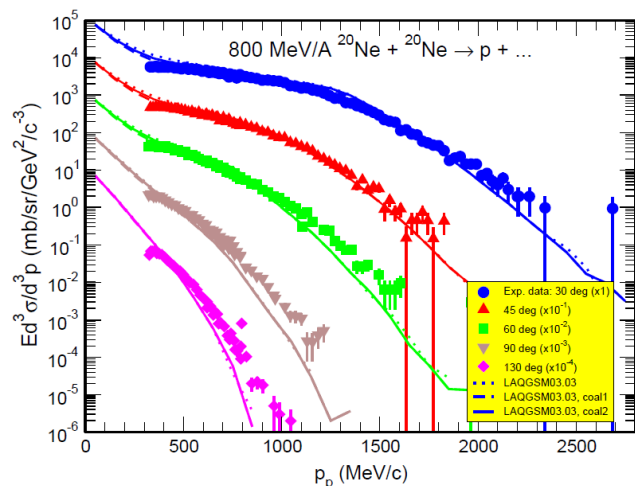
- n and p emitted during cascade
- These can “coalescence” into fragments up to ^4He , presently
- We will investigate allowing coalescence of larger fragments and update, if needed, the coalescence model

8. Replace the Preeq in LAQGSM

- LAQGSM uses almost the same preequilibrium models as CEM
- We will update these to reflect our CEM preequilibrium upgrades
- Verification and Validation

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Our preliminary results with an upgraded version of the coalescence model used in LAQGSM03.03 show a much better agreement with spectra of energetic complex particles from the reaction 800 MeV/nucleon $^{20}\text{Ne} + ^{20}\text{Ne}$ measured at the Bevatron/Bevalac at the Lawrence Berkeley Laboratory and published in: S. Nagamiya et al., Phys. Rev. **C24** (1981) 971; M.-C. Lemaire et al., Lawrence Berkeley Laboratory Report LBL-8463, 1978.

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9. Extend GENXS option of MCNP6

- Presently, GENXS allows us to tally spectra only up to ^4He
- Modify this to allow tally spectra of arbitrary products
- Verification and Validation how GENXS works for LF

10. Replace upgraded CEM and LAQGSM modules in MCNP6

- Replace the CEM and LAQGSM modules in MCNP6 with our upgrades and improvements
- Replace the standard GENXS module of MCNP6 with the extended version allowing us to tally arbitrary products
- Verification and Validation of the improved MCNP6

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Publications and Conferences

Past:

- Kerby, L. M., S. G. Mashnik, A. J. Sierk, “Preequilibrium Emission of Light Fragments in Spallation Reactions,” Proc. 2013 International Conference on Nuclear Data for Science and Technology (ND2013), March 4-8, 2013, New York, USA, to be published in Nuclear Data Sheet.
- Mashnik, S. G., L. M. Kerby, K. K. Gudima, A. J. Sierk, “Production of Energetic Light Fragments in Spallation Reactions,” Proc. 2013 International Nuclear Physics Conference (INPC 2013), June 2-7, 2013, Firenze, Italy, to be published in European Physical Journal Web of Conferences.

In progress:

- Kerby, L. M., S. G. Mashnik, A. T. Tokuhiro, “Production of Energetic Light Fragments with Expanded Cascade Exciton Model (CEM),” ANS Summary, to be presented at June 2014 American Nuclear Society Annual Meeting, LANL Report, LA-UR-14-20425, to be published in Transactions.
- Proton-induced reactions summary paper (Nuclear Physics A, 2014)
- Fermi Break-up and coalescence investigation summary paper (NIM A or NIM B, 2015)

Future:

- Summary paper, at conclusion of the project (Physical Review C, 2016)
- 2015 and 2016 conference proceedings

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Limitations

- Focusing only on preequilibrium (not upgrading evaporation models or the cascade models);
- Focusing on proton-, neutron-, and heavy-ion-induced reactions (no pion- or gamma-induced reactions);
- Where possible, new code will be written in Fortran 90 or 2003, but the bulk of the CEM code will remain in Fortran 77;
- The availability of experimental data for the emission of energetic LF from various targets and energies is not abundant; therefore our parameterization of γ_β for some emitted light fragments will be based on few experimental results

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Skills and Tools Required

- Knowledge of Spallation Reactions. Resources: **Stepan Mashnik**, "Handbook of Spallation Research" by D. Filges and F. Goldenbaum, Wiley-VCH, ISBN 978-3-527-40714-9, and available literature
- Fortran Programming Capability. I have these skills presently;
- Physics Analysis Workstation Proficiency. Resources: internet tutorials and **Konstantin Gudima**
- Mathematical modeling methods. Resources: **Ruprecht Machleidt**, **Francesca Sammarruca**, and available literature
- Numerical Interpolation and Extrapolation Methods. Resources: **Forrest Brown**, **Arnold Sierk**, and available literature
- Expertise in CEM and LAQGSM codes. Resources: **Stepan Mashnik**, **Arnold Sierk**, **Konstantin Gudima**, and available literature
- MCNP6 Modification Procedures. Resources: **Stepan Mashnik**, **Forrest Brown**, **Larry Cox**, and available literature

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Timeline

Table 1: Timeline

	2014				2015				2016			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Proton-induced reactions		X										
Neutron-induced reactions			X									
γ_β model analysis				X								
γ_β code modifications						X						
Fermi break-up						X						
Coalescence							X					
LAQGSM							X					
GENXS								X				
MCNP6									X			
Dissertation Defense										X		

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Summary

- ***Original Research:*** Expand preequilibrium processes models to include emission of light fragments and create systematics (or mathematical model) for generalization across arbitrary reactions
- Upgrading the MEM has been completed;
- Promising results have been obtained;
- More research remains:
 - More reactions need to be analyzed;
 - γ_β model development;
 - Fermi break-up and coalescence investigations
 - Implementation within LAQGSM and MCNP6
 - Extending the GENXS module in MCNP6
- I have the resources needed to complete this project

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